

07 JUNE 2017



# RCM STUDIES TO ENABLE GASOLINE-RELEVANT LOW-TEMPERATURE COMBUSTION



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Project ID # ACS054

FY2017 DOE Vehicle Technologies Office Annual Merit Review

Advanced Combustion Engine R&D

Wednesday, June 7, 2017

Program Managers: Gurpreet Singh, Leo Breton

**This presentation does not contain any proprietary, confidential or otherwise restricted information**

# OVERVIEW

## Timeline

- Project started FY 2011
- Project directions and continuation reviewed annually, and in FY 2017 VTO Lab Call

## Budget

- Project funded by DOE / VTO
  - FY 2015 funding: \$500 k
  - FY 2016 funding: \$490 k
  - FY 2017 funding: \$370 k

## Barriers

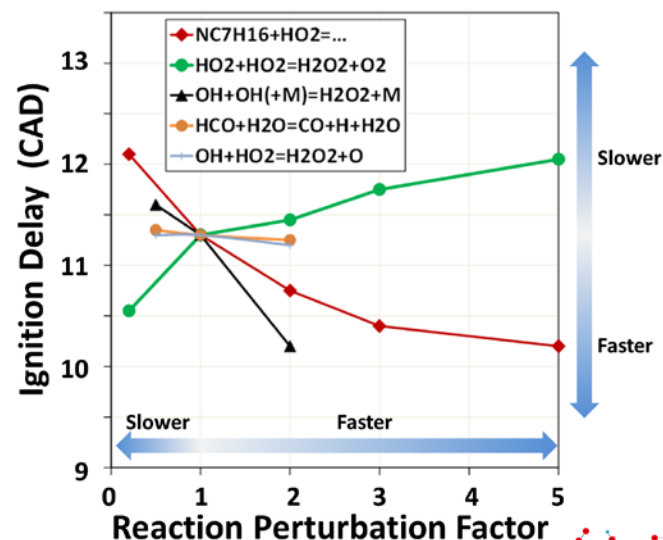
- Lack of fundamental knowledge of advanced combustion engine regimes
- Lack of modeling capability for combustion and emission control

## Partners

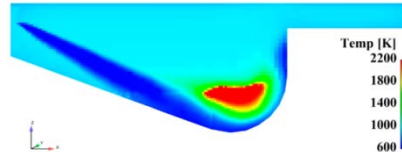
- ANL – Lead, Goldsborough (PI)
- LLNL – gasoline surrogate model, simulation tools
- KAUST, Chevron – fuels, fuel models
- SNL – RD5-87 gasoline, HCCI engine data
- International RCM Workshop

# OBJECTIVES AND RELEVANCE TO DOE

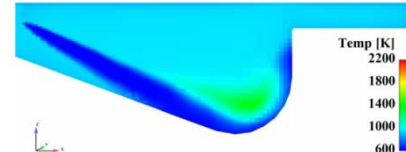
- Acquire fundamental data, and help develop / validate / refine chemical kinetic and relevant models for transportation-relevant fuels (conventional and future gasolines, diesels and additives) at conditions representative of advanced combustion regimes, leveraging collaborations with BES-funded groups, and researchers across the broader community.
- Predictive simulations with these models, which require low associated uncertainties, could be utilized to overcome technical barriers to low temperature combustion (LTC), and achieve required gains in engine efficiency and pollutant reductions.



doi:10.1021/jz400874s






$\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$



# PROJECT MILESTONES

FY 2017

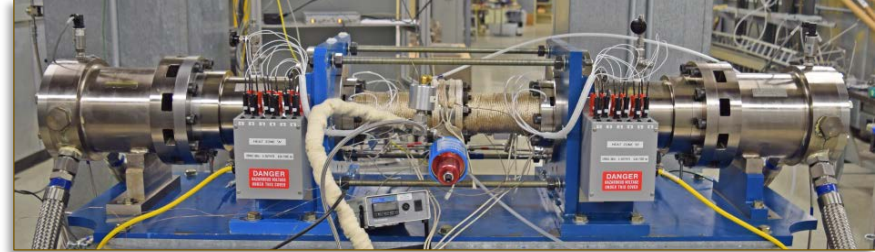
Task	Milestone	Status
1	Acquire ignition measurements for multi-component surrogate blends to mimic 'neat', and ethanol-blended gasolines (E0–E30). Evaluate, quantify performance of surrogate formulation approaches	
2	Acquire ignition measurements for full boiling-range gasoline, RD5-87 (an E10 gasoline), collaboration with SNL LTGC engine	FY17–Q3
3	Identify fuel, mixture and operational parameters that control flame initiation, and evolution of mild ignition at RCM conditions using detailed simulations	
4	Identify and hierarchically rank RCM design parameters and/or operating protocol that influence ignition delay measurements via mining of RCM Workshop Characterization Initiative database	
5	Acquire ignition measurements of single-component aromatics, and binary blends with olefins to probe synergistic/antagonistic behavior	FY17–Q4
6	Extend UQ/GSA framework and investigation to consider additional targets beyond ignition delay times, including heat release rates	FY17–Q4

# PROJECT APPROACH

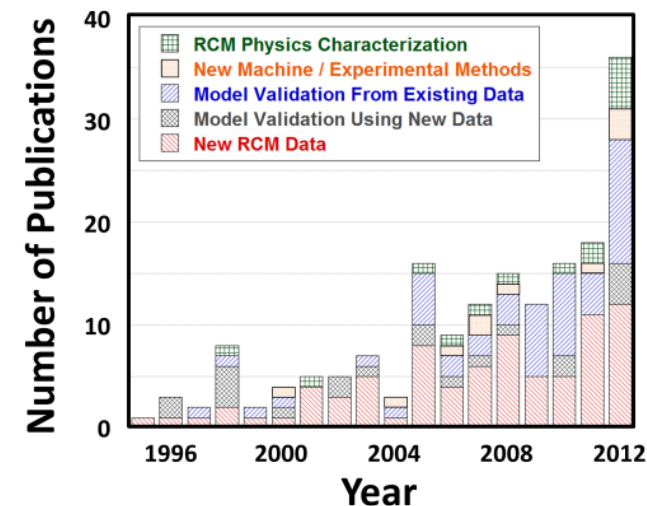
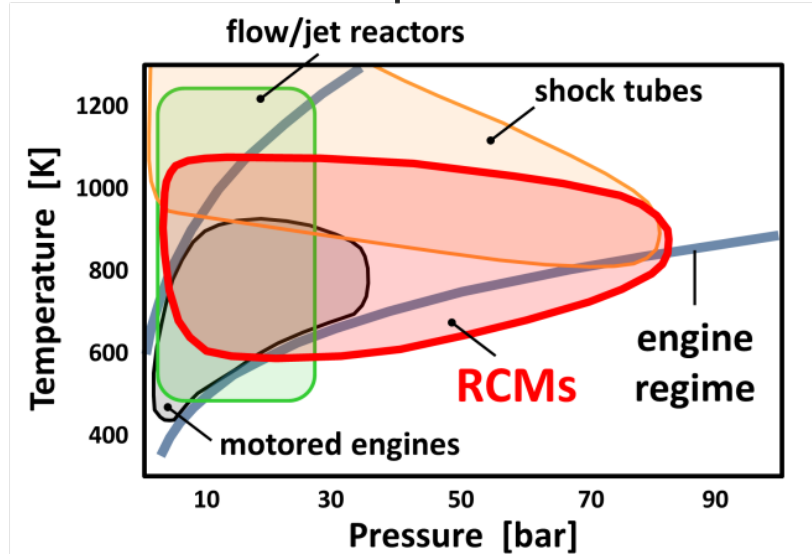


# PROJECT APPROACH

## Rapid Compression Machine



- Utilize ANL's twin-piston RCM to acquire autoignition data



- Employ novel data analysis tools and advanced diagnostics
  - Physics-based, reduced-order system model;
  - Developing diagnostics capabilities to better probe chemistry.
- Synergistically improve kinetic models using novel analysis techniques (e.g., UQ/GSA) and detailed calculations/measurements of sensitive processes (e.g., individual reaction rates)

# TECHNICAL ACCOMPLISHMENTS / PROGRESS

# PROJECT MILESTONES

## Twin-Piston Rapid Compression Machine

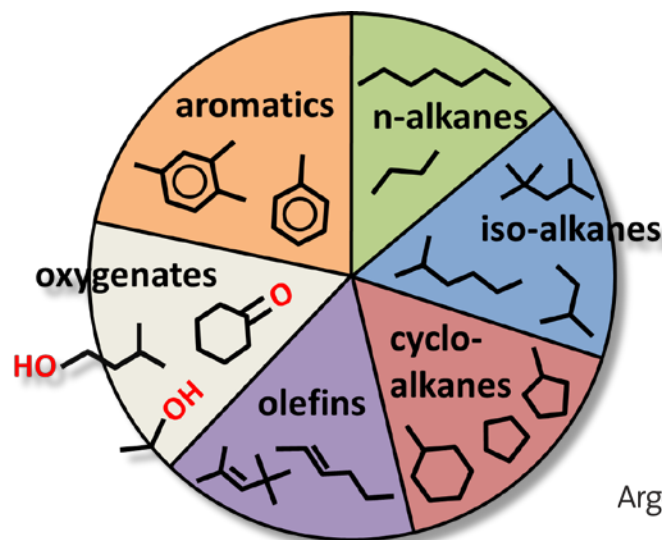
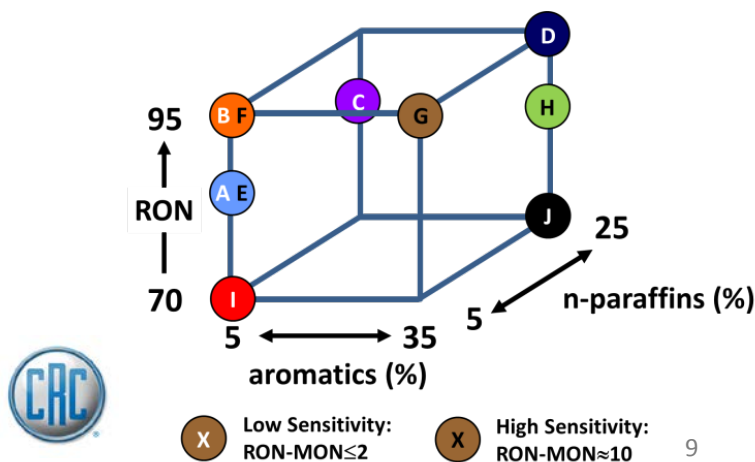
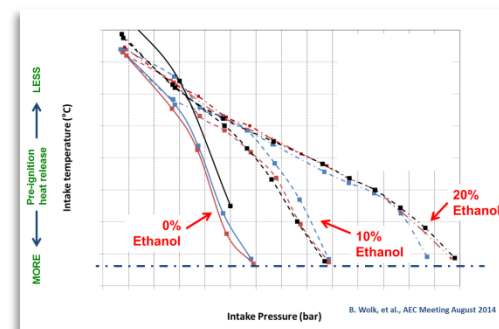
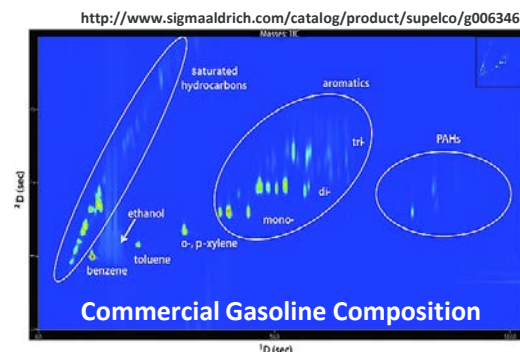
- Modifications and upgrades implemented since FY 2016 AMR to improve measurement capabilities
  - Designed / fabricated LVDT mounts for dynamic tracking of pistons during actuation to understand asynchronous piston behavior, assist with heat release analysis; final safety review underway;
  - Redesigned piston ringpacks for easier assembly, and to prevent seal disengagement; acquired new seals with increased wear resistance;
  - Designed / fabricated band heater for central portion of machine to ease assembly and achieve improved consistency between machine overhauls.
- Operational challenges exist
  - Synchronous twin-piston operation difficult to achieve; typically ~2-3 ms difference in actuation. Affects primarily short ( $\tau < 2$  ms) ignition delay times; can introduce noise / perturbations into heat release analysis, complicating quantification of LTHR.



# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Investigating Gasoline and Surrogates

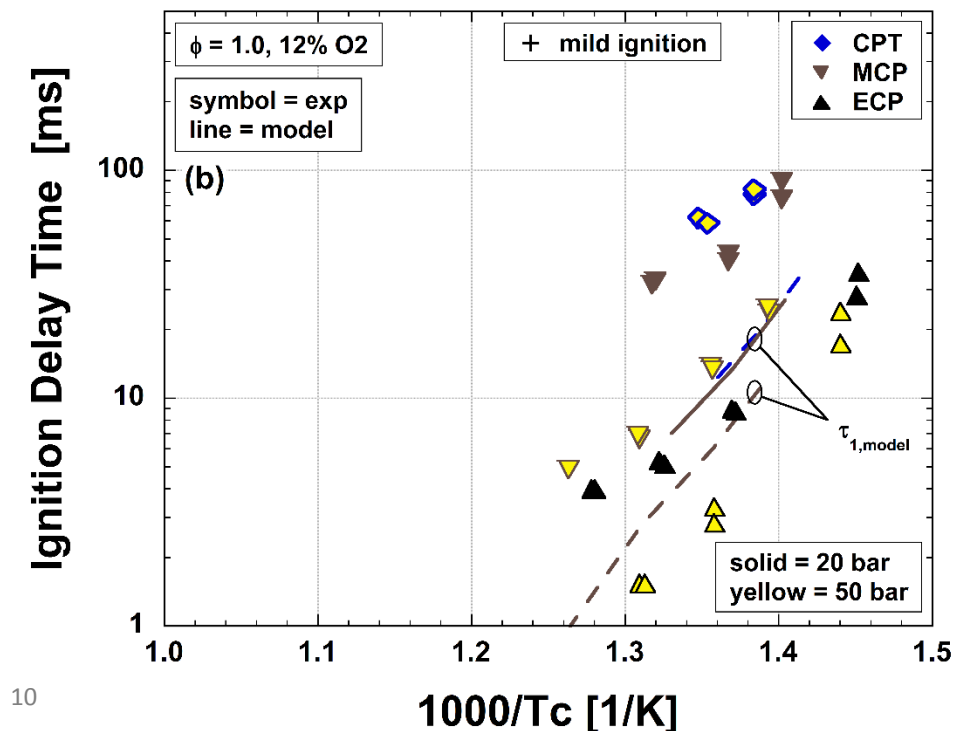
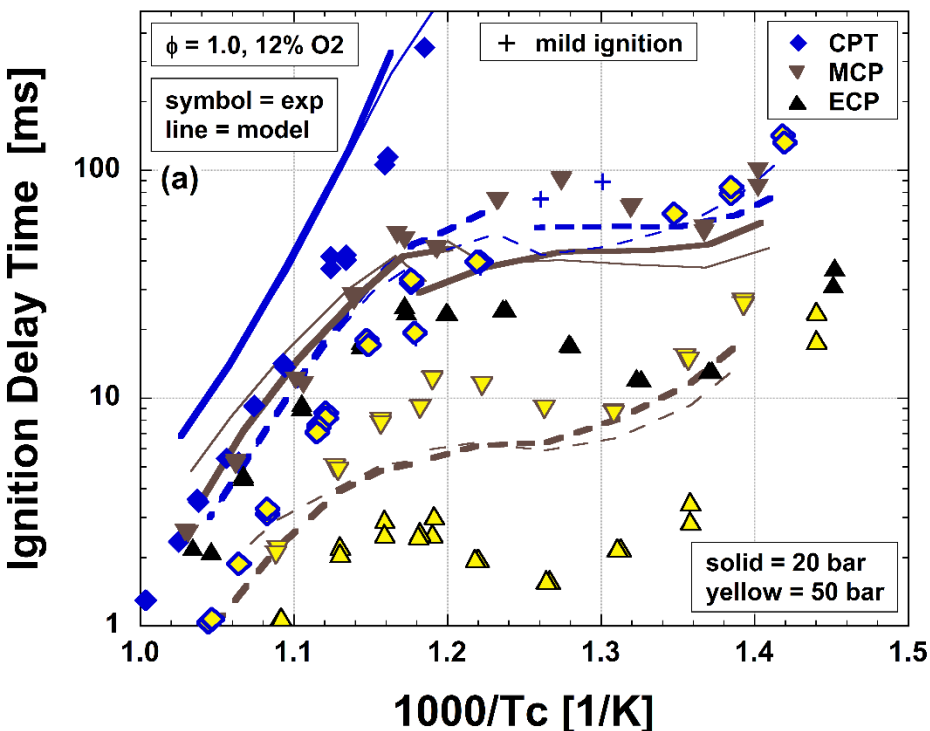
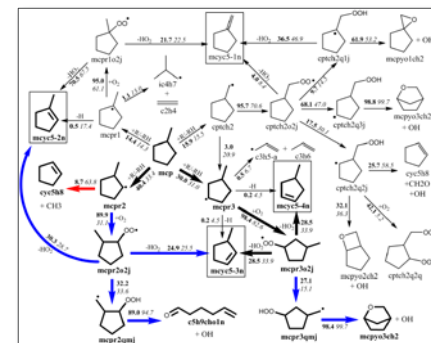
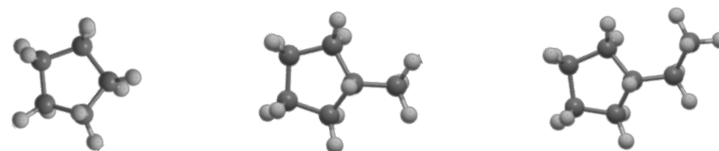
- Predictive modeling of LTC needed to guide design
  - Gasoline is complex, compositionally variant
    - How do these features affect LTC behavior, especially autoignition phenomena at low and intermediate temperatures ( $T = 600\text{--}1100\text{ K}$ )?
    - How can real fuels be represented by multiple-component (3-10) formulations?
    - Data are needed to compare autoignition behavior of real, full boiling range fuels with surrogates, including individual components, blends of these and mixtures with ethanol.



# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Surrogate Components

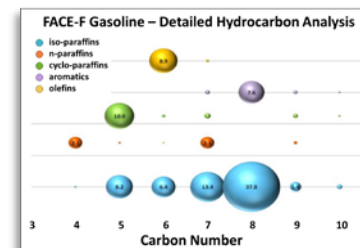
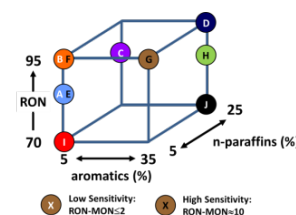
- 5-membered ring naphthenes
  - Acquired data for CP, MCP and ECP in FY15/16, at LTC conditions to quantify influence of ring substitution, temperature, pressure and dilution;
  - Assisting KAUST, LLNL with CP, MCP model evaluation, improvements.



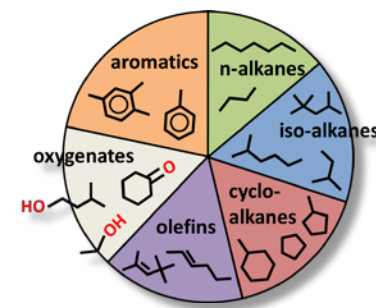
# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Task 1 – Gasoline / Ethanol Blends

- FACE-F used as representative gasoline
  - Composition, properties well-characterized;
  - Investigating various approaches to formulate multi-component surrogate mixtures, measuring influence of ethanol (blending levels of E0–E30) on autoignition chemistry; quantifying  $\tau$ , LTHR/ITHR changes.

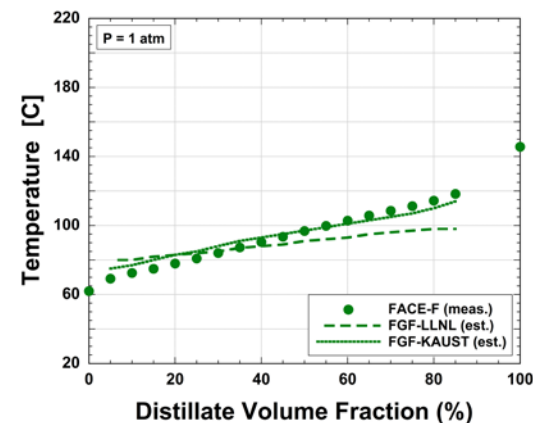


Property	FACE-F	PRF 91.5	TPRF-F	FGF-LLNL	FGF-KAUST
RON	94.4	91.5	94.4	93.8	93.6
MON	88.8	91.5	89.1	89.5	88.9
S	5.6	0	5.3	4.3	4.7
Density (g/mL)	707	694	755	712	707
H/C	2.13	2.25	1.84	2.06	2.12
Avg. MW (g/g-mol)	94.8	112.9	103.9	100.2	96.2
Branching Index	0.68	0.55	0.69	0.51	0.50



Component	PRF 91.5	TPRF-F	FGF-LLNL	FGF-KAUST
n-Butane	0	0	0	6.9
2-Methyl butane	0	0	0	9.8
2-Methyl hexane	0	0	0	7
Cyclopentane	0	0	14	15.8
1,2,4-Trimethyl benzene	0	0	0	8.4
1-Hexene	0	0	14	8.4
n-Heptane	9.5	11.1	7	0
2,2,4-Trimethyl pentane	90.5	49.1	53	43.7
Toluene	0	39.8	12.1	0

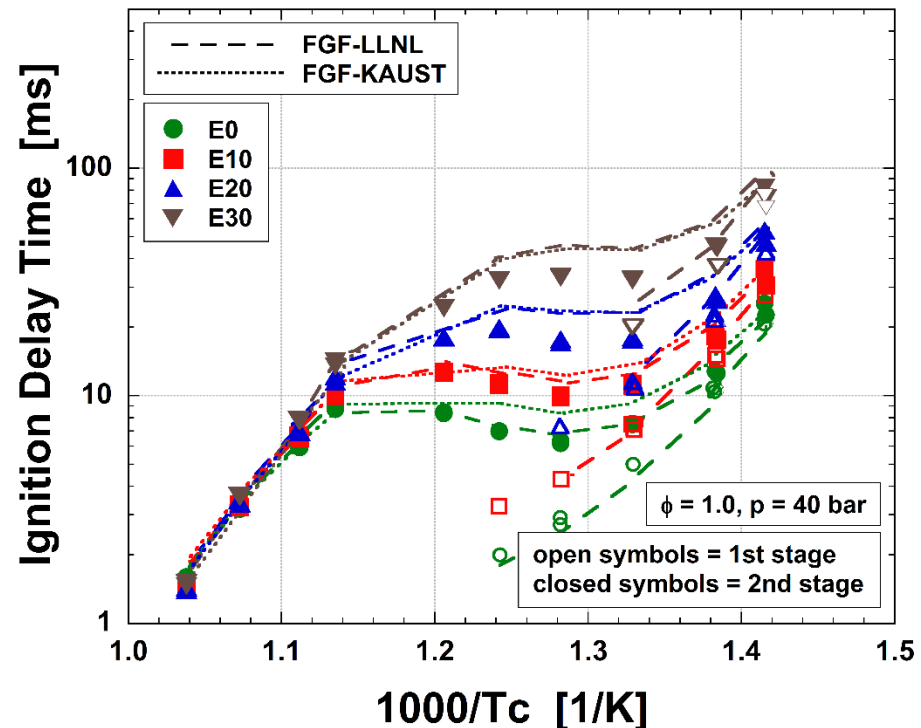
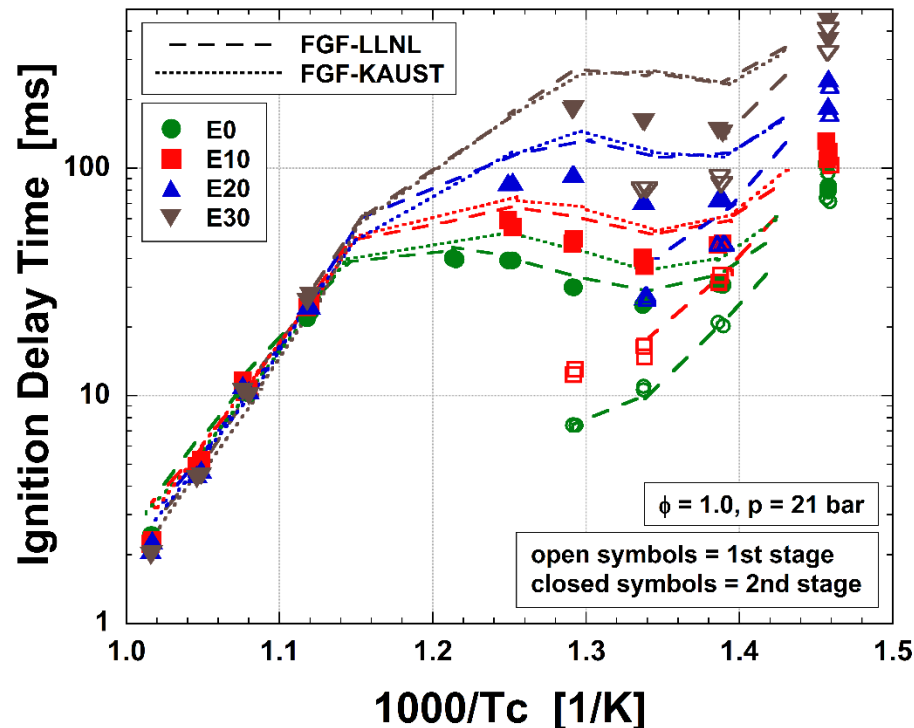
Mole percentages of components in surrogate blend



# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Task 1 – Gasoline / Ethanol Blends

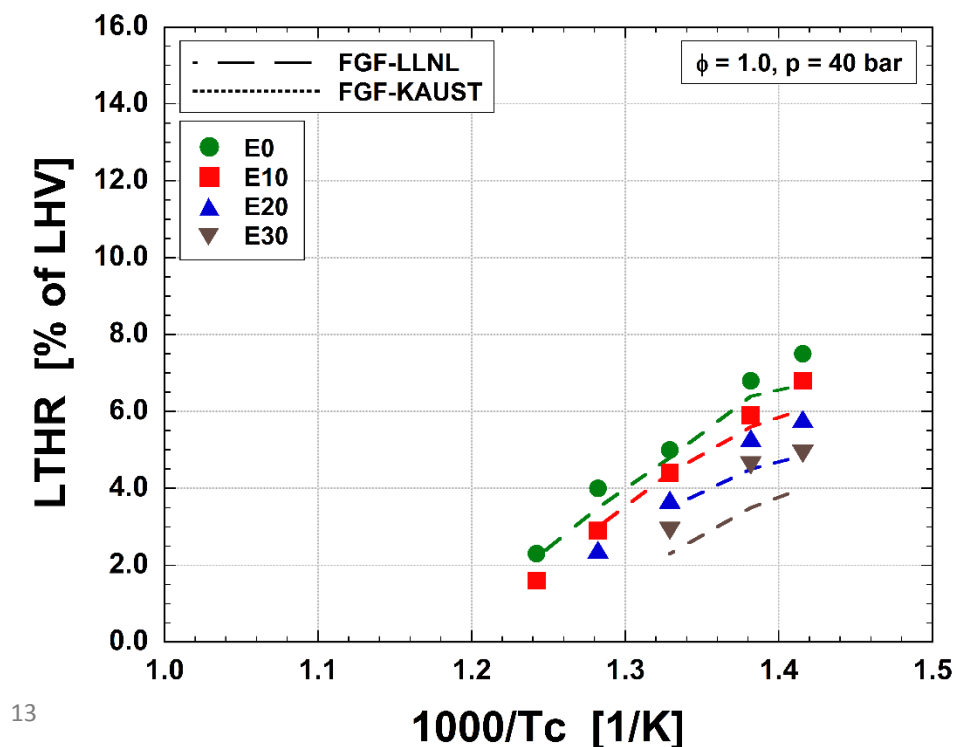
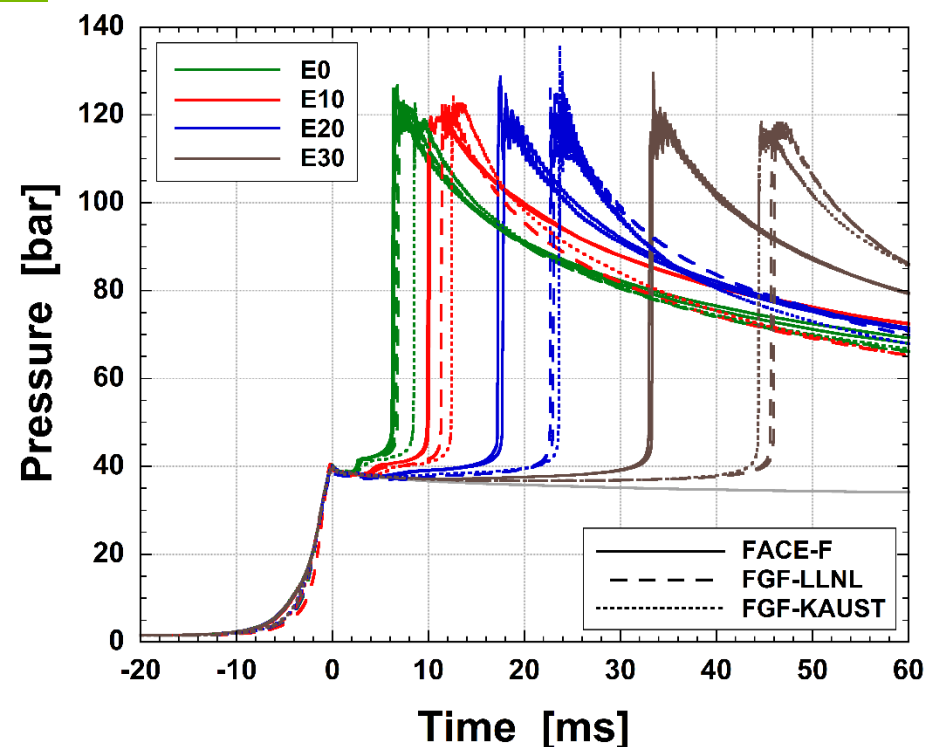
- Autoignition behavior experimentally measured for FACE-F, surrogates
  - $T_c = 690\text{--}980\text{ K}$ ,  $P_c = 21, 40\text{ bar}$ ,  $\phi = 1$ , E0–E30;
  - As with full boiling range gasoline, influence of ethanol blending into surrogates is most significant at NTC, low-temperature conditions;
  - FGF-LLNL very closely matches 1<sup>st</sup> stage and main ignition times of FACE-F, but more perturbed by ethanol addition than FACE-F, FGF-KAUST.



# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Task 1 – Gasoline / Ethanol Blends

- Experimental examination of low-temperature reactivity highlights differences in response to ethanol blending
  - Timing and extent of LTHR evolve differently for full boiling range gasoline, and the 5-, 7-component FACE-F surrogates;
  - Measurements highlight need to improve surrogate formulation methodologies, so that neat fuels properly respond to component blending.

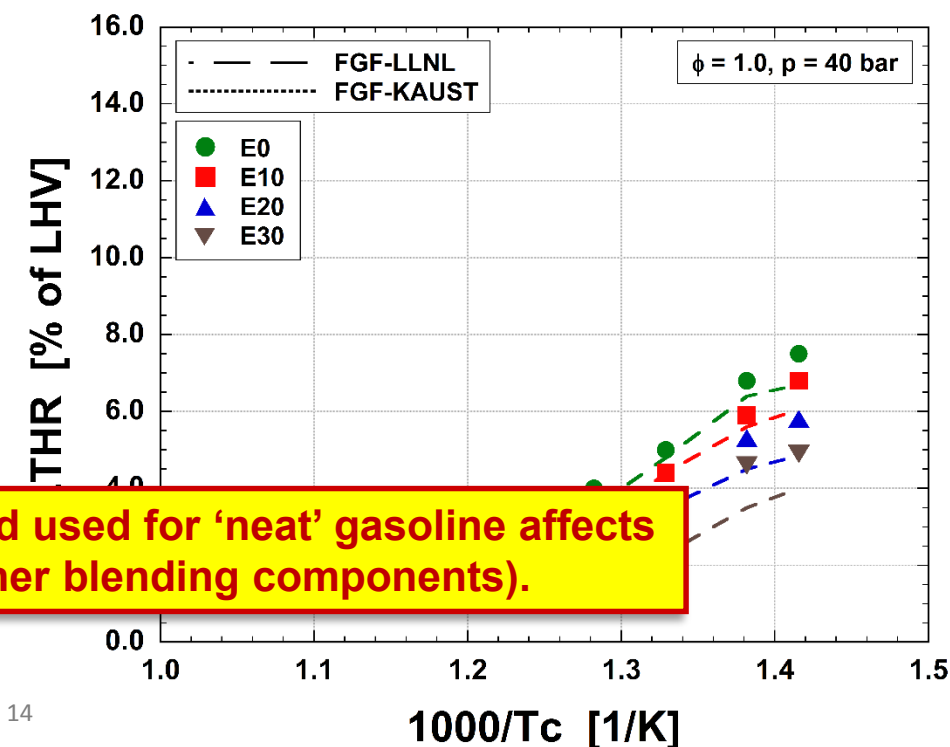
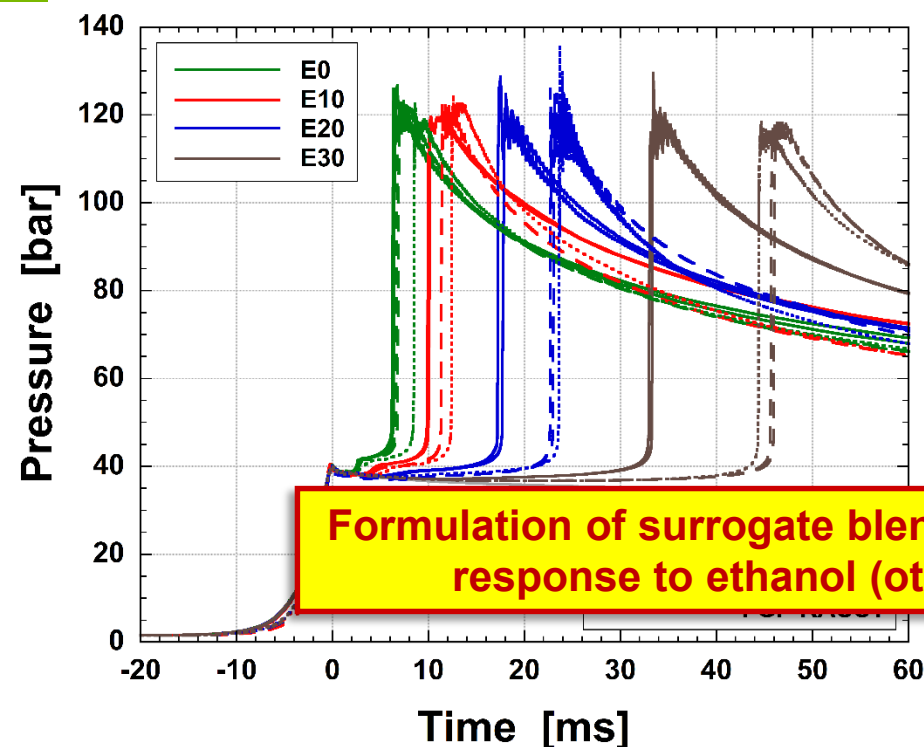




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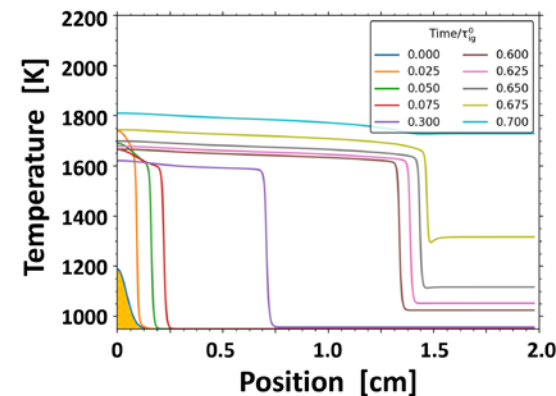
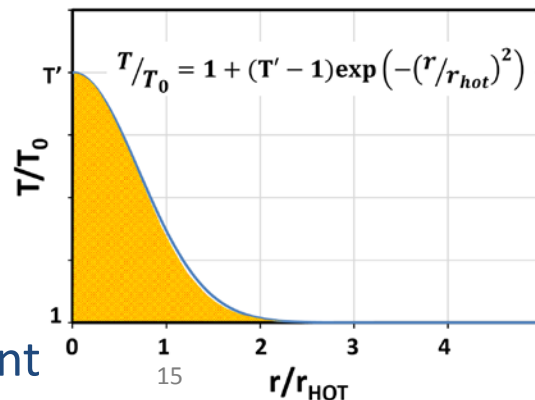
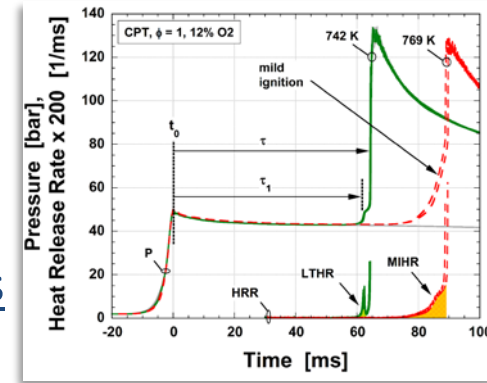


Formulation of surrogate blend used for 'neat' gasoline affects response to ethanol (other blending components).

# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Task 3 – Mild Ignition – Understanding / Mitigation

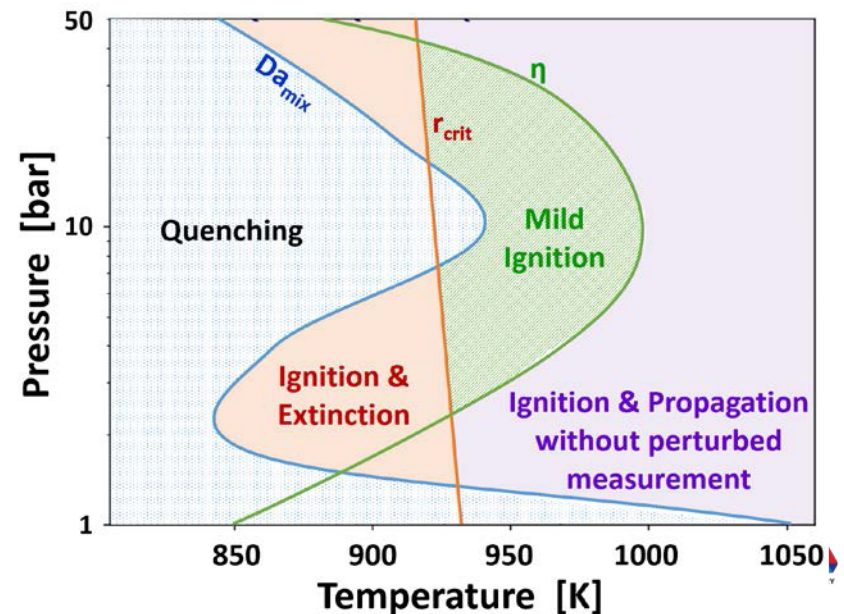
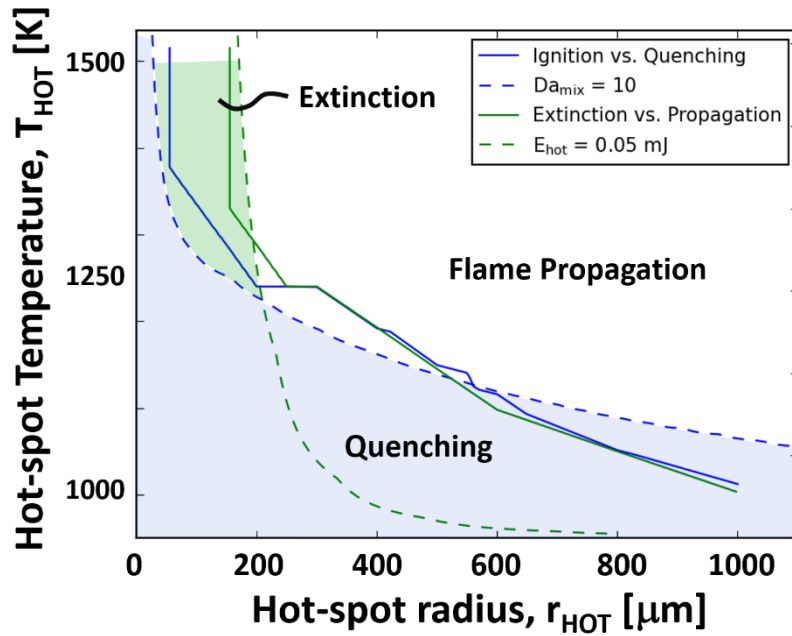
- Mild ignition can occur in some tests where flame kernels form, and consume reacting mixture via deflagration (observed in RCMs, shock tubes, ...)
  - Kernels can be initiated from particles, oil or hot-spots
  - These data are not easily compared to kinetic models.
- Efforts undertaken to understand processes of kernel initiation / growth due to hot-spots (e.g., caused by thermo-acoustic effects, etc.)
  - Identify fuel, mixture and operational parameters that influence these;
  - Determine how experimental protocol could be used to mitigate events.
- Detailed parametric simulations conducted using DNS code (ASURF)
  - Hot-spot characteristics
    - $T' = 1.01\text{--}1.90$
    - $r_{\text{HOT}} = 25\text{--}1000\ \mu\text{m}$
  - Syngas ( $\text{CO}/\text{H}_2 = 80/20$ )
    - $\phi = 0.2\text{--}0.5$
  - 800–1120 K, 1.5–15 bar
  - Modified transport, diluent



# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Task 3 – Mild Ignition – Understanding / Mitigation

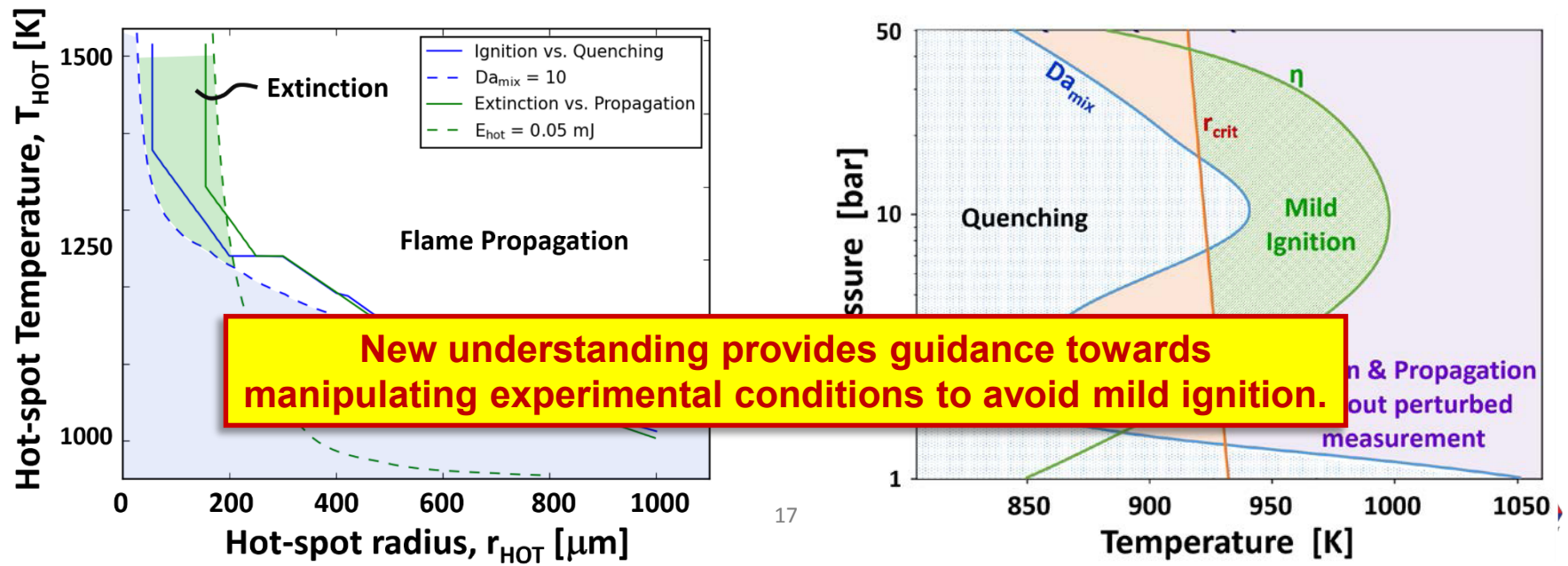
- Simulations reveal dynamics of hot-spots – quenching/ignition, flame propagation/extinction over a range of local conditions
  - Quenching controlled by mixing Damköhler number;
  - Extinction controlled by critical stretch rate of flame kernel.
- New regime diagram for fuel, mixture and operational conditions
- DNS results utilized towards reliably predicting, detecting mild ignition events, without need for optical identification of flames



# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Task 3 – Mild Ignition – Understanding / Mitigation

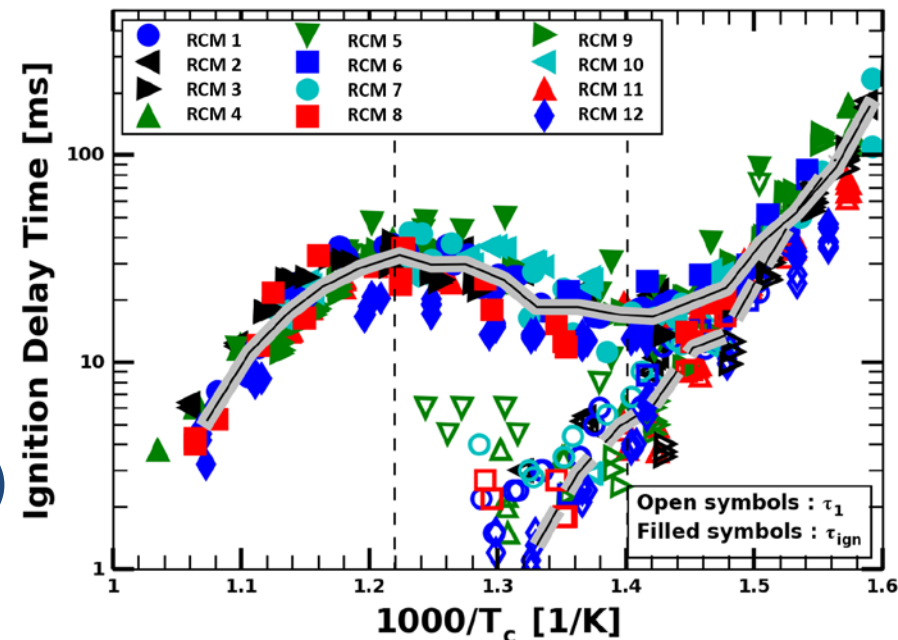
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# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Task 4 – RCM Workshop

- Data from many RCM facilities used for kinetic model development
- RCM Workshop Characterization Initiative created to better understand and quantify facility influences on measured ignition delay times
  - What are primary causes of machine-to-machine differences?
  - Are there ways to modify design / operating protocol for more consistency?
  - What are useful techniques to normalize datasets?
- Fifteen facilities worldwide
  - Included wide diversity of machine configuration / operating protocol;
  - iso-Octane/'air',  $T_c = 630\text{--}965\text{ K}$ ;
  - Non-reacting and reacting tests
    - 700+ experimental points
  - Raw pressure-time data post-processed with single script, using consistent definitions ( $t_0$ ,  $t_{50}$ ,  $\tau_{ign}$ ,...)
  - Extensive details of geometries provided to facilitate analysis.

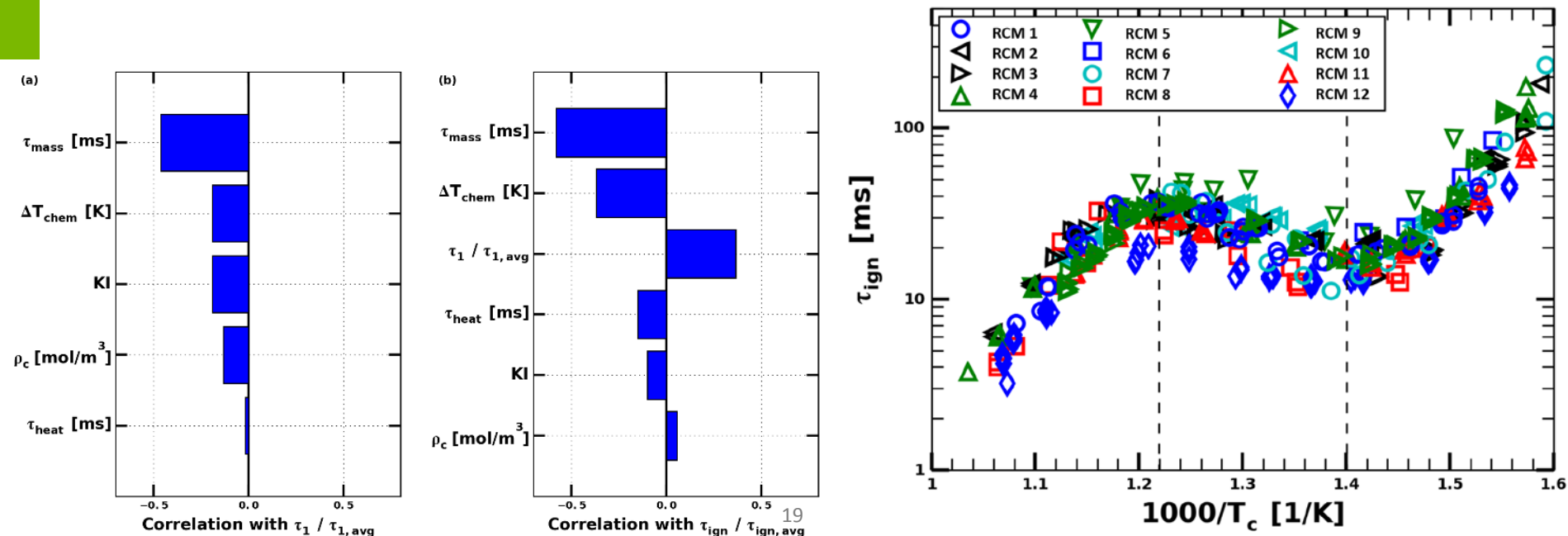




# TECHNICAL ACCOMPLISHMENTS / PROGRESS

## Task 4 – RCM Workshop

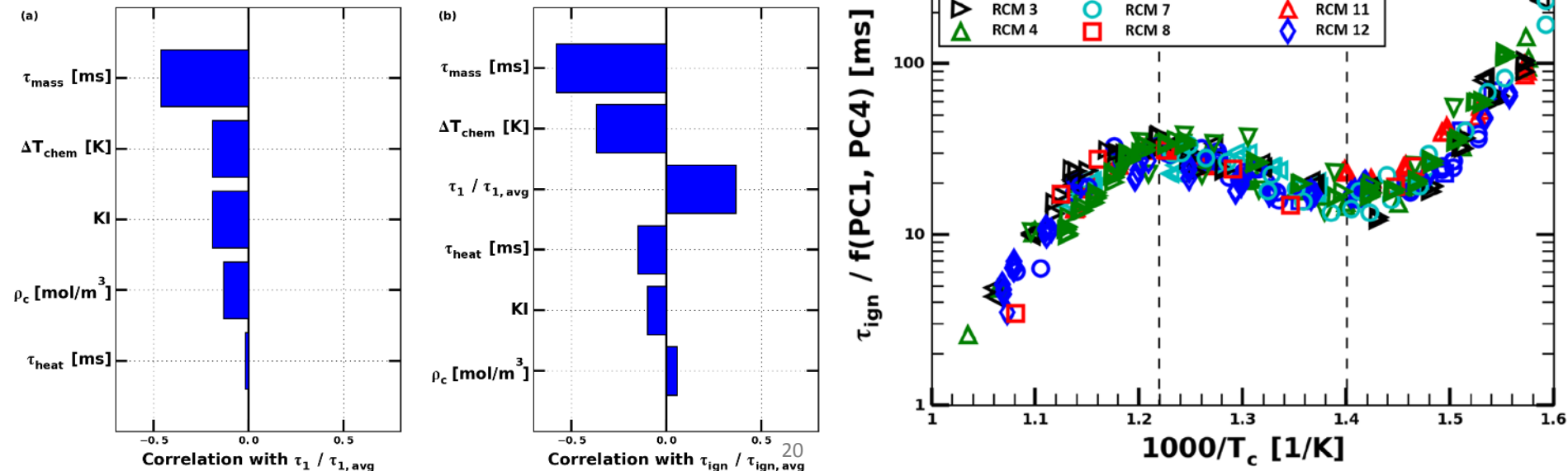
- Data mining techniques employed to recognize patterns in dataset
  - Ascribe scatter to particular design / operating characteristics;
  - Hierarchically identify most important facility influences;
  - Scale measurements against principal coordinates.
- Analysis reveals unique insight, not available without large collaboration
  - Under conditions investigated, machine-to-machine variations primarily due to: (i) piston seating mechanism, (ii) configuration of piston crevice;



# TECHNICAL ACCOMPLISHMENTS / PROGRESS

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  - Scale measurements against principal coordinates.
- Analysis reveals unique insight, not available without large collaboration
  - Under conditions investigated, machine-to-machine variations primarily due to: (i) piston seating mechanism, (ii) configuration of piston crevice;
  - Scatter can be reduced,  $F = 1.65 \rightarrow 1.4$ .



# RESPONSE TO REVIEWER COMMENTS

- The project is very instrumental towards acquiring RCM data to support improvements in chemical kinetic modeling for relevant fuels for the transportation industry, which is important in the design of new, more efficient engines that will reduce petroleum usage. Fundamental ignition delay data have been collected extensively for gasoline surrogate components, and gasoline/ethanol blends, but the project should be careful to not repeat what has been done in the literature. The gasoline surrogate model needs to be improved to capture the low-temperature, high-pressure region, and thus higher ambient pressure data might be needed. It is unclear however, how the RCM-generated data can be compared to operating engine environments where turbulence, swirl, and liquid phases set the initial conditions for in-cylinder processes, while the in-cylinder conditions cannot be simulated from a first-principles approach with the same high fidelity modeling that the RCM is amenable to. Furthermore, there are certain engines/conditions where ignition can occur within the multiphase domain of the injected spray. The project team is very good, with very good external collaborations, however it appears that these may only be through information exchange, and the teams are encouraged to work closely to interpret the data at a deeper level.
  - The project team at ANL coordinates closely with the LLNL groups focused on chemical kinetic modeling, and advanced numerical tools. This extensive collaboration is leveraged to ensure that RCM experiments target fuels and conditions needed to address model deficiencies, and thus model improvement, while questions raised by the data are pursued through development and application of new computational tools and algorithms, such as techniques to conduct sensitivity analyses on heat release rates over a range of fuels and operating conditions.
  - The RCM data presented in FY16's AMR identified new approaches to directly comparing against HCCI engine data where a constant combustion phasing perspective was adopted. This technique allows very good correlation between the complex reciprocating device, and the well-characterized RCM where direct evaluation of chemical kinetic models towards these trends can be undertaken. Certainly, the current experiments are not intended to directly replicate the complex, transport dominated environment of spray combustion; that would be closer to IQT experiments.

# COLLABORATIONS

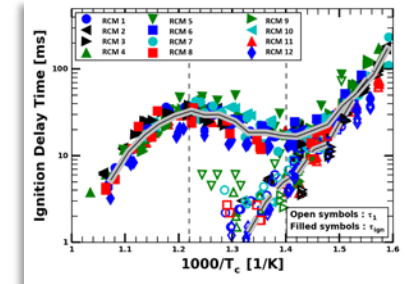
## Ongoing Interactions (Inside / Outside VTO)

- **DOE Working Groups on LTC engines**: share data at meetings of AEC MOU
- **CRC FACE Working Group**: participate in meetings; testing of AVFL-20 fuels
- **ANL**: gasoline LTC engine towards fuel metric development; refine UQ/GSA approaches and target reactions for mechanism improvement
- **LLNL**: gasoline model development / validation; formulation of gasoline surrogates; ToolKit development / testing
- **KAUST / Chevron**: provide FACE fuels; mechanism development
- **SNL**: LTGC engine data with RD5-87; tests with surrogate molecules
- **Trinity College Dublin**: functional-group basis for surrogate formulation
- **Other organizations**: Princeton/Peking Universities (ASURF); NUI Galway (kinetic models, student exchange); Northeastern University (mechanism integration, diagnostics/analysis); Vrije Universiteit Brussel (reduced-order physical models); U. Leeds (UQ/GSA approaches); Danmarks Tekniske Universitet (PhD exchange student).

# COLLABORATION

## Community-wide Activities

- ANL-led, International RCM Workshop to better understand LTC phenomena using RCMs, especially autoignition chemistry, turbulence-chemistry interactions, etc.
  - Participation includes experimentalists, modelers, theoreticians
  - Establishing consensus for ‘Best Practices’
    - Approaches for reporting / analyzing / comparing data
    - Approaches for simulating the experiments
    - Uncertainty quantification for experiments and modeling
    - Regimes of overlap with other experimental devices
  - 4<sup>th</sup> Workshop to be held 27 July 2018 at Trinity College Dublin, IRELAND (in conjunction with International Combustion Symposium)





# REMAINING CHALLENGES / BARRIERS

- Understanding and representing the autoignition characteristics of full boiling range fuels, blending with ethanol, etc., via multiple-component (3-10) surrogate mixtures requires improved capabilities to formulate surrogates, considering new methods and surrogate components;
- Improvements to gasoline surrogate model require deeper understanding of mechanism behavior, and uncertainties associated with low temperature chemistry pathways of base model;
- Ignition delay time and preliminary heat release are integrated metrics for ignition chemistry, constraints exist with their utility; additional diagnostics, like heat release rates, measurement of chemical intermediates, etc., could improve development / validation efforts;
- Mild ignition, which can be initiated due to local perturbations in the gas temperature, can complicate autoignition measurements under some conditions; application of new insight across range of fuels needed in order to develop as approaches to mitigate this.

# PROPOSED FUTURE WORK

## FY 2017 and beyond

- Proposed future work is subject to change based on funding levels
- Physical testing of multi-component surrogates (FACE-F, etc.), leveraging interactions with LLNL / others, to improve robustness of formulations
  - Utilize various techniques / targets to select component molecules, blending ratios, including blends with ethanol;
  - Understand chemical kinetic interactions between neat fuel and ethanol;
  - Conduct tests with individual components and full boiling-range gasolines.
- Conduct RCM tests with RD5-87 (E10 certification gasoline)
  - Coordinate with SNL to target LTGC engine conditions (T, P,  $\phi$ , EGR);
  - Coordinate with LLNL to formulate and test surrogate blends for RD5-87.
- Ignition measurements of surrogate aromatics, binary blends with olefins to probe synergistic/antagonistic behavior
  - Coordinate with LLNL for component selection, model development
- Extend UQ/GSA to additional targets such as heat release rates, reaction intermediates

# PROPOSED FUTURE WORK

## FY 2017 and beyond

- Proposed future work is subject to change based on funding levels
- Conduct tests with CRC AVFL-20 fuels
  - Coordinate with MIT, NREL and AVFL-30 committee to better understand / interpret measurements across RCM, IQT and spark-ignition engine platforms considering knock-limited performance
- Conduct tests / modeling with unique molecules, e.g., cycloheptadiene, in collaboration with Combustion Chemistry group at SNL CRF
  - Quantify influence of peroxide intermediates, e.g. QOOH, which have been directly measured by CRF, on autoignition behavior at engine-relevant conditions ( $T$ ,  $P$ ,  $\phi$ ,  $\%O_2$ ) via RCM measurements and kinetic modeling

# SUMMARY

- Objective
  - Acquire data, validate / improve models for transportation-relevant fuels
- Project Approach
  - Utilize ANL's RCM and novel analysis tools, leverage expertise of BES-funded researchers to synergistically improve predictive models
- Technical Accomplishments / Progress
  - Acquired data to understand autoignition behavior of multi-component surrogate blends for gasolines, including ethanol blends (E0–E30);
  - Identified fuel, mixture and operational parameters controlling mild ignition;
  - Hierarchically identified facility influences on RCM measurements.
- Collaborations
  - National labs, universities and industry; International RCM Workshop
- Future Work
  - Testing with gasoline surrogate components, blends and full boiling range gasolines at engine-relevant (T, P,  $\phi$ , EGR) conditions;
  - Advances / improvement in UQ/GSA, covering additional targets.

An aerial photograph of the Argonne National Laboratory campus, showing various buildings, parking lots, and a large circular structure, all rendered in a blue-tinted, semi-transparent style.

# THANK YOU